Alignment and orientation in the electron-impact excitation of H- and He-like ions

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(Received 16 July 1990; revised manuscript received 26 December 1990)

The alignment and orientation parameters of excited states are theoretically studied for the electron collision with H-like and He-like ions. With the use of the distorted-wave method, those parameters are calculated for the excitation of the $2\,^1P$ and $2\,^3P$ states of He-like ions with $Z=3,8,\infty$ and the $2p$ state of H-like ions with $Z=2,6,\infty$. Here Z is the nuclear charge of each ion. The dependence of the parameters on the scattering angle and the collision energy is examined along the isoelectronic sequences. When compared at the same collision energy in threshold units, the parameter as a function of the scattering angle is not much changed along each isoelectronic sequence.

I. INTRODUCTION

Electron-impact excitation of atomic ions is one of the fundamental processes in plasmas. Detailed study of the process is of importance in various fields such as astrophysics and laboratory plasma physics. Differential cross sections (DCS's), in particular, give a good insight into the excitation mechanism. In previous papers the present authors reported a systematic study of the DCS's for H-like and He-like ions.[1-4]

Alignment and orientation parameters (AOP's) are another of the quantities which provide detailed information on the mechanism of collisional excitation of atoms and ions. Those parameters describe as completely as possible the state of an excited target after a collision. For neutral atoms, a large number of studies have been already published on AOP's (see recent reviews[5,6] and the papers cited therein). To the best of our knowledge, only two papers reported a calculation of AOP's for electron-impact excitation of atomic ions.[7,8] Both of the papers made only a Coulomb-Born calculation (without electron exchange) for H-like ions, i.e., the simplest calculation on the simplest target. Although they give some interesting results, a more comprehensive study is desirable for the AOP's of ions.

In the present paper, which is to some extent a continuation of our previous works,[1-3] we present a systematic theoretical study of AOP's for H- and He-like ions. For the former ions, the transition $1\,^2S-2\,^2P$ is considered and for the latter $1\,^1S-2\,^1P,2\,^3P$ transitions are studied. To obtain scattering amplitudes, use is made of the distorted-wave method developed by Itikawa and Sakimoto.[9] For neutral H and He, a distorted-wave approximation has been found useful to study AOP's at intermediate energies.[10-12] The present distorted-wave method has already been applied to the calculation of DCS's for He-like ions.[1,3] Together with those results of DCS's, the present calculation of AOP's provides a detailed picture of the collision process between an electron and an ion. Furthermore, the present study, especially the study along an isoelectronic sequence, would be helpful in understanding the behavior of the AOP's in the collision of an electron with neutral atoms.

II. THEORETICAL METHODS

A. Alignment and orientation parameters

The collision plane is chosen here to be xz plane with the z axis being along the direction of the incident electron. The scattering amplitude for the excitation of a magnetic sublevel m is denoted by a_m. For simplicity, the relativistic effect and the effect of nuclear spin are not considered in the present paper. The atomic units are used unless otherwise stated.

For the excitation of P state of He, the following two parameters are usually used to describe the details of the excited state:

$$\lambda=\frac{|a_0|^2}{|a_0|^2+2|a_1|^2}\ , \tag{1}$$

$$\chi=\arg(a_1/a_0)\ . \tag{2}$$

We can use these parameters also for He-like ions, but, according to the suggestion by Andersen, Gallagher, and Hertel,[5] we adopt here the orientation parameter $\langle L_y\rangle$ and alignment angle γ. For He or He-like ions, those parameters are defined by[5]

$$\langle L_y\rangle=-2[\lambda(1-\lambda)]^{1/2}\sin\chi\ , \tag{3}$$

$$\tan 2\gamma=-\frac{2[\lambda(1-\lambda)]^{1/2}}{2\lambda-1}\cos\chi\ . \tag{4}$$

If the initial state is an s state as in the present problem, $\langle L_y\rangle$ represents the angular momentum transferred to the target during the collision. The angle γ denotes the direction of the major axis of the electron cloud with respect to the z axis.

An electron collision with H-like ions is explicitly spin dependent. Here we study, however, only the spin average of the amplitudes

$$\lambda=\frac{\langle|a_0|^2\rangle}{\sigma}\ , \tag{5}$$

$$R=\frac{1}{\sigma}\mathrm{Re}\langle a_1 a_0^*\rangle\ , \tag{6}$$

$$I=\frac{1}{\sigma}\mathrm{Im}\langle a_1 a_0^* \rangle \tag{7}$$

with $\sigma=\langle |a_0|^2\rangle+2\langle |a_1|^2\rangle$. Here $\langle\ \rangle$ means the spin average defined by

$$\langle a_m a_m^* \rangle=\tfrac{1}{4}(a_m^s a_m^{s*}+3a_m^t a_m^{t*}) , \tag{8}$$

where s and t refer to the singlet and triplet amplitudes, respectively. With the use of these spin-averaged amplitudes, the parameters $\langle L_y \rangle$ and γ for H-like ions are given by[5]

$$\langle L_y \rangle=-2\sqrt{2}I , \tag{9}$$

$$\tan 2\gamma=-\frac{2\sqrt{2}R}{2\lambda-1} . \tag{10}$$

B. The distorted-wave method

In the present paper, each scattering amplitude is calculated with the distorted-wave method developed by Itikawa and Sakimoto.[9] The method [called the distorted-wave with exchange-approximation (DWXA)] uses as a distortion potential the spherical average of the electrostatic potential formed by the target ion in its initial state. This distortion potential is adopted for the calculation of the distorted waves both in the initial and in the final states. Electron exchange is taken into account, but only for the interacting two electrons. No unitarization is made. Further details of the method are given in the previous paper.[9]

In principle, any potential can be chosen as the distortion potential (see a general discussion of the distorted-wave approximation[13]). It is almost impossible to determine mathematically which potential is the best. Only a comparison with experiment or more accurate theory may select the best potential. In the case of $2\,^1P$ excitation of He, Beijers *et al.*[14] concluded from a comparison to experiment that the present choice of the potential (i.e., the ground-state potential for both the initial and final channels) is not sufficiently adequate for the calculation of γ parameter. In the case of He-like ions, however, such a comparison cannot be made. For highly charged ions, the Coulomb potential dominates so much that the difference in the distortion potential may be expected to cause little difference in the cross section. Thus we have adopted here the simplest choice of the distortion potential.

The present work for He-like ions is an extention of the previous DWXA calculation[1,3,9] of the integral and differential cross sections. The integral cross sections obtained by the present method, especially for the P-state excitation, were found in good agreement with those of a more accurate calculation.[9] It is worth noting that the DWXA gives a reliable cross section even for a singlet-triplet transition, particularly for a highly charged ion. As in the previous papers, the target state in the present calculation is represented by a configuration-interaction (CI)-type wave function produced by the computer code CIV3.[15] The configurations considered are $1s^2$, $2s^2$, $2p^2$, $1s2s$ for $1\,^1S$ and $1s2p$, $2s2p$ for $2\,^1P$ and $2\,^3P$ states. The detailed form of the wave functions is given in the paper by van Wyngaarden, Bhatia, and Henry.[16] As the paper shows, the calculated values of the energy difference and the oscillator strength are in good agreement with experiment. For the H-like ions, this is the first application of the DWXA.

III. RESULTS AND DISCUSSION

Here the AOP's are calculated and compared along an isoelectronic sequence with varying nuclear charge Z. To complete the comparison, the AOP is calculated also in the limit $Z\to\infty$. In the limit, the electron-electron interaction can be ignored when compared to the electron-nucleus interaction. The distorted wave becomes the Coulomb wave for the point charge Z. Furthermore, if the length is scaled by Z^{-1} and the energy by Z^2, the wave equation for the incident electron has the same form, and thus the scattering amplitude multiplied by Z^2 is a universal function of the collision energy divided by Z^2. In the limit $Z\to\infty$, the wave function of the target

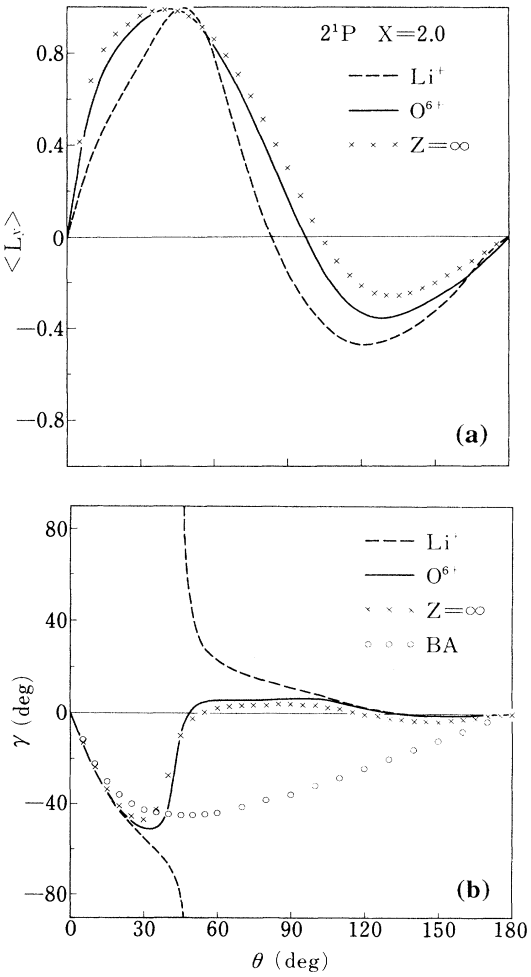

FIG. 1. Alignment and orientation parameters $\langle L_y \rangle$ (in a.u.) and γ as a function of scattering angles for the $2\,^1P$ excitation of He-like ions, calculated at $X=2.0$ (i.e., twice the threshold). Open circles (b) denote γ calculated in the plane-wave Born approximation, which does not depend on nuclear charge.

ion is a simple product of the hydrogenic one and the excitation energy increases as Z^2. Since the AOP's are given by a ratio of the relevant scattering amplitudes, they are independent of Z in the limit $Z \rightarrow \infty$, when compared at a given value of the collision energy X in threshold units (i.e., $X = E/\Delta E$, ΔE being the excitation energy). In Secs. III A and III B the AOP's calculated are shown along the He and the H isoelectronic sequences, respectively. They are compared at the same value of X so that they are expected to be not much different from each other, at least for highly charged ions.

A. He-like ions

The parameters $\langle L_y \rangle$ and γ calculated for the excitation of $2\,^1P$ state of the He-like ions with $Z = 3$, 8, and ∞ are compared in Fig. 1 at $X = 2.0$. Figure 2 shows a similar result but for $X = 4.0$. Some aspects of the calculation in the limit $Z \rightarrow \infty$ are described above, and more details are given in the previous paper.[1]

The behavior of each parameter does not much change depending on Z, except for γ of Li^+ at $X = 2.0$. In particular, the alignment angle in the small-scattering-angle region (i.e., $\theta < 20°$) has almost the same value for different ions. In the plane-wave Born approximation, γ is given by[5]

$$\tan\gamma^{BA} = \frac{\sin\theta}{\cos\theta - C} \tag{11}$$

with $C = [E/(E-\Delta E)]^{1/2} = [X/(X-1)]^{1/2}$. If X is given, γ^{BA} is a universal function independent of ion species. In Fig. 1, γ^{BA} for $X = 2.0$ is also plotted for comparison. As is seen from the figure, the present result for γ is successfully explained by γ^{BA} in the region of small scattering angles. As is mentioned above, the θ dependence of the parameter γ for Li^+ at $X = 2.0$ is different from that for more highly charged ions. It rather resembles the corresponding γ parameter for neutral He at 40 eV ($X = 1.89$) summarized in a recent review.[5] In this case, therefore, Li^+ remains to have some amount of neutral characteristics. This kind of feature is also seen in some cases of the differential cross section previ-

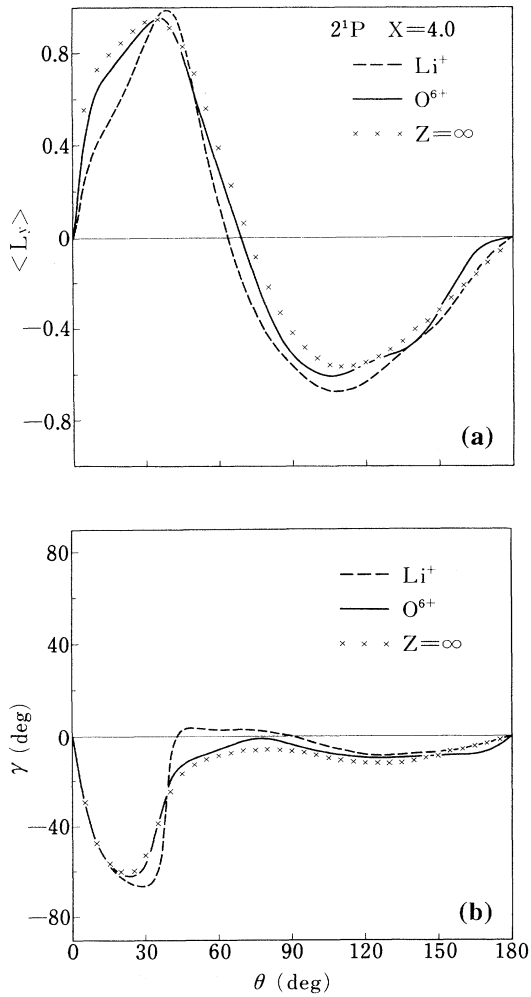

FIG. 2. Same as Fig. 1, but at the collision energy $X = 4.0$.

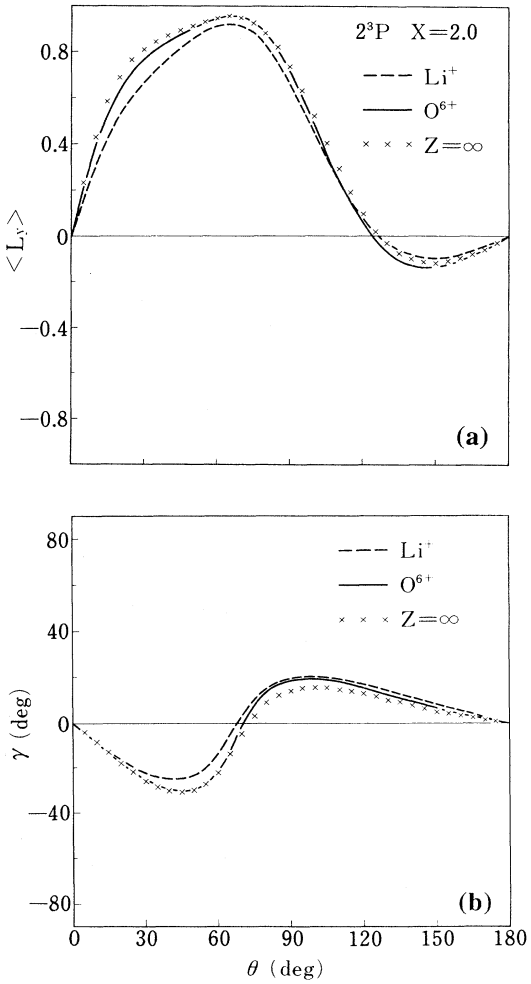

FIG. 3. Same as Fig. 1, but for the excitation of $2\,^3P$ state of He-like ions.

ously studied.[1,3]

According to the classical grazing-incidence model,[17] an effective attractive (repulsive) force between the incident electron and the target atom makes $\langle L_y \rangle$ positive (negative). The present result of $\langle L_y \rangle$ at small scattering angles is consistent with this model. That is, the attractive Coulomb force between the electron and the ion determines the behavior of $\langle L_y \rangle$. The Coulomb force is so different depending on the ionic charge that it does not follow the simple scaling along Z. In fact, a remarkable difference in $\langle L_y \rangle$ for different ions is noticeable in the small-angle region in Figs. 1 and 2. As in the case of He,[11] the behavior of $\langle L_y \rangle$ in the large-angle region cannot be simply understood by the classical model. That may be a result of complicated interference of the contributions of many partial waves. It should be noted that the plane-wave Born approximation gives $\langle L_y \rangle$ to be identically zero in the s-p transition.[5] (Madison, Csanak, and Cartwright[7] suggested that the classical model is not adequate to explain the electron scattering from He and H, but later Lin *et al.*[18] showed that, from the study of scattering of electrons, positrons, protons, and antiprotons from He and H, only the electron scattering at large angles is inconsistent with the classical model. It is interesting, therefore, to apply the model to some other systems like the present one.)

Figure 3 shows the parameters $\langle L_y \rangle$ and γ for the excitation of $2\,^3P$ state of the He-like ions with $Z=3$, 8, ∞ calculated at $X=2.0$. We calculated those parameters also at $X=4.0$ but do not show the result here because its qualitative behavior does not change from the result at the lower energy.

The most interesting point to note is that the Z scaling is more satisfactory for $2\,^3P$ than for $2\,^1P$. The excitation of the former state is caused only through electron exchange. Electron exchange has a large effect at a collision relatively close to the target ion, where the force of nuclear charge dominates. This may be at least a partial explanation of less deviation from the Z scaling in the $2\,^3P$ excitation. Further evidence of the dominance of the nuclear Coulomb force is that $\langle L_y \rangle$ in the $2\,^3P$ excitation is positive almost all over the scattering angles.

During the present study, it has been found that the computation of the distortion potential was not correctly carried out in some cases in the previous study of DCS's for the $2\,^1P$ excitation.[3] This error affects only the case of small nuclear charge. Here in Fig. 4 we present the corrected result of the DCS for the $2\,^1P$ excitation of the He-like ions with $Z=3$, 8, ∞ calculated at $X=2.0$. [From the same argument as given at the beginning of this section, the scaled cross section (i.e., the DCS multiplied by Z^4) are compared at a given value of X.] When compared to the previous calculation (Fig. 4 in Ref. 3),

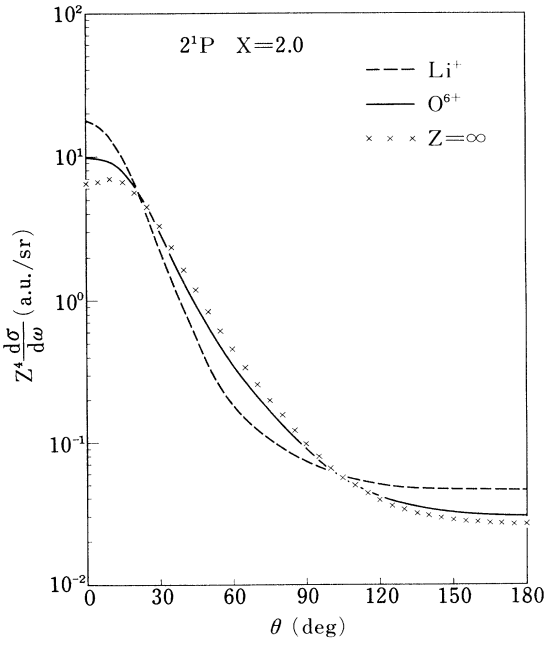

FIG. 4. Differential cross sections multiplied by Z^4 for the $2\,^1P$ excitation of He-like ions at the collision energy $X=2.0$.

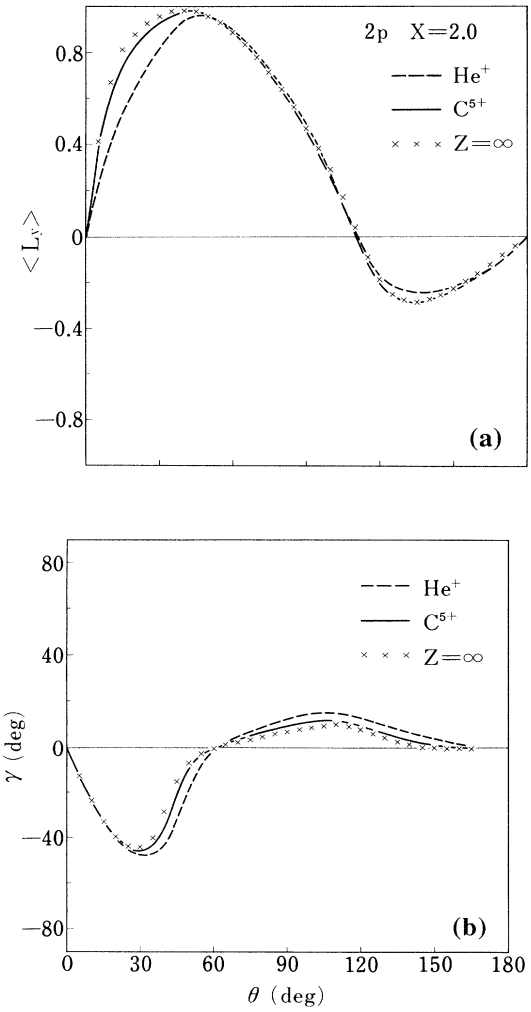

FIG. 5. Alignment and orientation parameters as a function of scattering angles for the $2p$ excitation of H-like ions calculated at $X=2.0$.

only the large-angle region of the curve for Li^+ is changed.

B. H-like ions

Figure 5 shows the parameters $\langle L_y \rangle$ and γ for the excitation of $2p$ state of the H-like ions with $Z=2$, 6, ∞, calculated at $X=2.0$. The qualitative feature of the parameters for the $2p$ excitation in the H-like ions is similar to that for the $2\,^1P$ excitation in the He-like ones. The Z scaling is much more satisfactory for H-like ions than for He-like ions. This may be the reflection of the fact that the former ions have only one bound electron.

As is mentioned in the Introduction, two groups[7,8] have reported the AOP for the excitation of $2p$ states of H-like ions. Both of them based their calculation on the Coulomb-Born (CB) approximation. They ignored the effect of electron exchange. In Fig. 6 we compare the AOP of He^+ obtained by the DW method to those by the CB approximation. Here we also show the result of the calculation with the CB approximation with electron exchange [i.e., the so-called Coulomb-Born-Oppenheimer (CBO) method]. The present CB and CBO methods are based on the formulation by Burgess, Hummer, and Tully.[19] The scattering amplitude in the CBO approximation is obtained simply by antisymmetrizing the final-state wave function in the CB amplitude. More details of the calculation are given in a previous paper.[2] The CB result shown here is in complete agreement with the corresponding one obtained by Jain *et al.*[8]

It is interesting to note in Fig. 6 that the result of the CB calculation has an angular dependence qualitatively similar to that of the DW one, while the CBO calculation results in an angular dependence different from those two methods. This tendency can also be seen in the differential cross section. Figure 7 compares the DCS for the excitation of $2p$ state of He^+ calculated with the three methods: the DWXA, CB, and CBO. In the small-angle region, the CBO result agrees better with the DWXA one than the CB value. In the large-angle region, however, only the CBO cross section has a minimum as a function of θ. It is well known[20] that some ambiguity is involved in the way of incorporating an electron-exchange effect in the Born-type approximation. The CBO method is a natural extension of the CB one and becomes exact in the limit $Z \to \infty$. The present feature of the CBO result shown in Figs. 6 and 7 suggests, however, that the electron exchange cannot be taken into account in a consistent manner in the CBO method in the case of low-charged ions.

One significant difference between the results of the DW and the CB calculations is seen in γ at a large

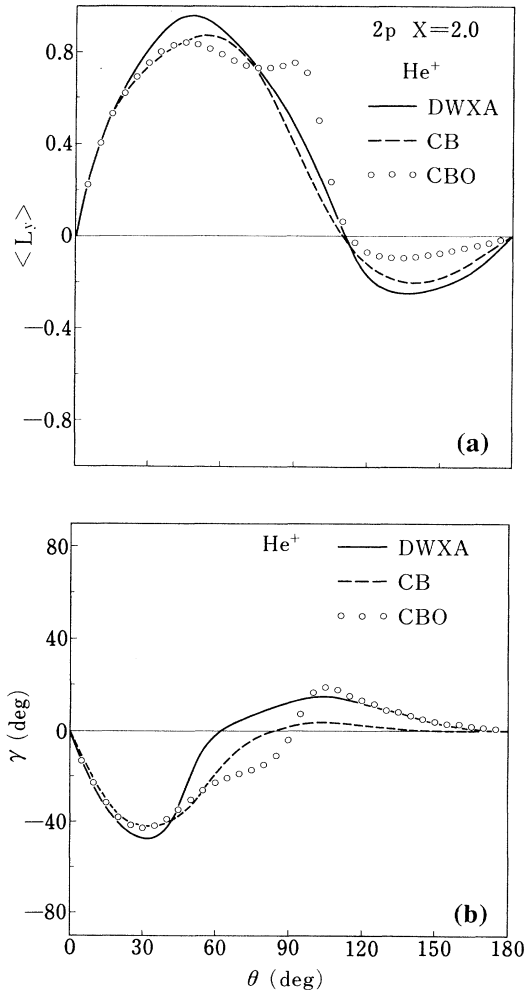

FIG. 6. Comparison of the alignment and orientation parameters for the excitation of $2p$ state of He^+ calculated in the distorted-wave with exchange-approximation method (DWXA) and the Coulomb-Born approximations with (CBO) and without (CB) electron exchange at the collision energy $X=2.0$.

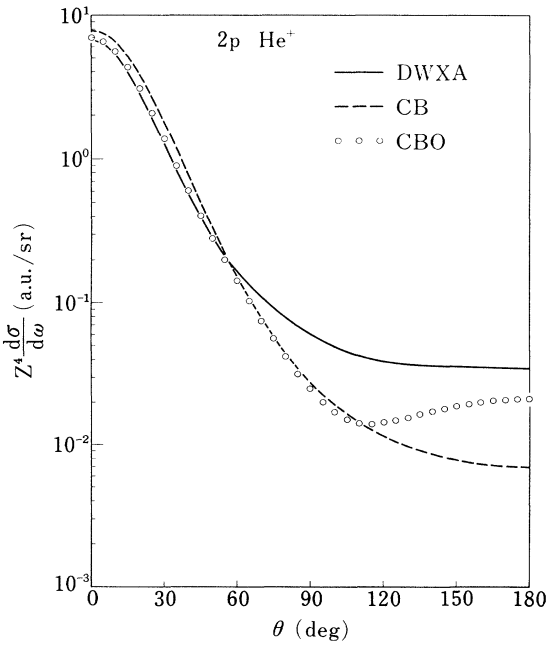

FIG. 7. The same comparison as in Fig. 6, but of the differential cross sections for the excitation of $2p$ state of He^+.

scattering angle. The γ calculated by the DWXA has a positive value in the region, while the corresponding result in the CB approximation is almost equal to zero. This difference should be ascribed to the effect of the distortion of the wave of the scattered electron.

IV. CONCLUSION

In the present paper, a systematic study was made on the alignment and orientation parameters (AOP's) in the electron-impact excitation of atomic ions. The excitation of $2\,^1P$ and $2\,^3P$ states was considered for He-like ions and the excitation of $2p$ state for H-like ions. The calculation of the scattering amplitudes was done with the distorted-wave method developed by Itikawa and Sakimoto. For H-like ions, a comparison was made with the calculation in the Coulomb-Born approximation with and without electron exchange.

The parameters thus calculated were compared along each isoelectronic sequence. When compared at a given collision energy in threshold units, the parameters for different ions have, in most cases, a similar shape and magnitude as a function of scattering angles. This confirms the universal behavior of the AOP's for ions, which was first observed by Jain *et al.*[8] in their Coulomb-Born calculation of H-like ions. When we examine the result in more detail, a deviation from the universality is found in some cases. The deviation probably gives a clue to insight into the details of the mechanism of the excitation of ions.

There are no experiments to compare with the present calculation. The calculation of AOP can be extended to obtain the polarization of the emission radiated from the excited state of the target. Such a polarization may be of importance in laboratory or astrophysical plasmas and may be experimentally detectable.[21]

ACKNOWLEDGMENTS

The present authors would like to thank S. Nakazaki, who provided them with the transition matrix elements calculated in the CB and CBO approximations. One of the authors (R.S.) would like to thank the Institute of Space and Astronautical Science for the hospitality provided to him during his stay there.

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